Pretending to Transport Radiation

An Overview of the Transport Methods Group, CCS-4, to the Division

Todd Urbatsch

Computer, Computational, and Statistical Sciences Division

June 28, 2006

LA-UR-06-4484

Outline

- Mission
- Types of radiation transport
- CCS-4 Software and Applications for radiation transport
- Issues
- Research
- Software Quality Engineering
- Existing and Potential Collaborations within the Division

Transport Methods Group CCS-4

Group Office

Todd Urbatsch, Group Leader
Scott Turner, Deputy Group Leader
Tina Maestas, Administrative Specialist
Dan Mahoney, Computer Technician

Monte Carlo

Todd Urbatsch, Team Leader
Mike Buksas
Jeff Densmore
Tom Evans, PL
Aimee Hungerford
Tim Kelley
Scott Mosher

Deterministic Radiation Transport

Scott Turner, Team Leader
Kent Budge
Jae Chang
Kelly Thompson, PL
Jim Warsa

Students

Erin Fichtl, UNM
Max Rosa, Penn State
Alex Maslowski, TAMU
Rick Gleicher, UNM
Teresa Bailey, TAMU

Linear Deterministic Transport

Randy Baker, Team Leader
Ray Alcouffe, Retired
Jon Dahl
Robert Ward

Students

Michael Reed, TAMU
Eric Baker, Oregon St.

Boltzmann Transport Equation

- Linear radiation transport equation for steady-state neutrons

$$\Omega \cdot \nabla \psi + \Sigma_t \psi = \iint \Sigma_s(\Omega' \to \Omega, \mathrm{E}' \to \mathrm{E}) \psi' \mathrm{d}\Omega' \mathrm{dE}' + \frac{\chi(E)}{k} \iint \nu \Sigma_f \psi' \mathrm{d}\Omega' \mathrm{dE}' + \mathrm{Q}$$

- Nonlinear radiation transport equation for thermal x-rays

$$\frac{1}{\mathrm{c}} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I = \sigma(B - I)$$

$$\mathrm{C_v} \frac{\partial T}{\partial t} = \frac{\partial E_{mat}}{\partial t} = \iint \sigma(I - B) \mathrm{d}\Omega \mathrm{d}\nu + Q$$

- With as many as seven dimensions of the transport equation and with 100s or 1000s of discrete variables per dimension, we devote our efforts to new methods, algorithms, and software that balance speed, accuracy, efficiency, robustness, and time-to-solution.

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Transport Methods Group

Mission

Provide the best numerical radiation transport capability to LANL and external customers*

*optimal

Spectrum of Activities

Methods	Algorithms	Software	Applications
R&D publish present	R&D publish present	design develop hardware, OS test, QA integrate	direct indirect via users experiments

Activities performed on the foundation of the computing environment.

CCS-4 Funding

- **ASC** **12 FTE**
  - Integrated Codes
    - Transport Project 7.0 FTE
    - Code Project A 1.5 FTE
    - Code Project B 1.0 FTE
    - Core Integrated Technologies 1.75 FTE
  - TN Burn Initiative 0.5 FTE
  - Hostile Environments 0.25 FTE
- **Weapons Supported Research** **2.5 FTE**
- **Emergency Response** **0.5 FTE**
- **Attribution** **0.25 FTE**
- **Work For Others** **0.1 FTE**
- **LDRD** **1.0 FTE**
  - Supernovae neutrinos
  - Coming out of the cosmic dark

Radiation Transport Applications

- Neutral particle, linear transport
  - Nuclear reactor simulations
    - Criticality (k-effective)
    - Isotope depletion
    - Shielding
    - Probability of Initiation
      - Also: subcritical experiments, reprocessing plants
  - Medical, e.g., brachytherapy
  - Oil well logging
  - Subcritical experiments
- Nonlinear transport of thermal x-rays
  - Inertial confinement fusion (ICF)
  - Z-Pinch machine at Sandia National Laboratory
  - Astrophysics

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Scaling the 7-Dimensional Mountain

- The transport equation has seven dimensions
  - 3 in space
  - 2 in angle
  - 1 in energy or frequency
  - 1 in time
  - Plus, coefficients depend on material temperature
- We devote our efforts to balancing speed, accuracy, efficiency, and time-to-solution.
- What can we get away with?
  - Diffusion: $\psi = A + B\Omega$?
  - 2, 1, or even 0 dimensions?
  - Gray?
  - Steady-state?
  - Equilibrium diffusion?

Computing Requirements

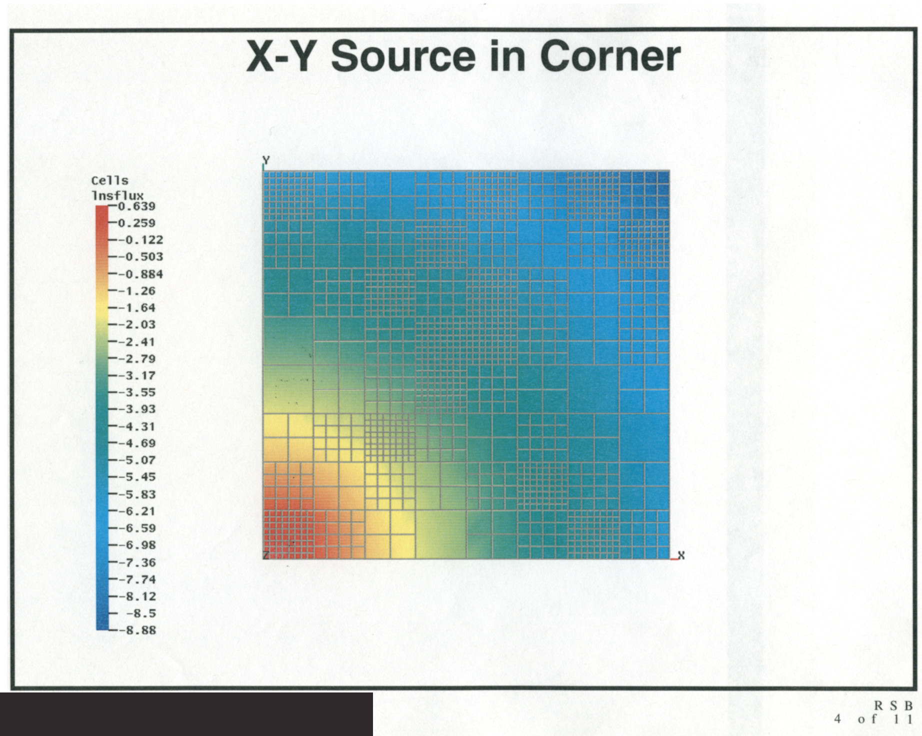
- Consider the memory and speed requirements
  - 1-100M spatial cells
  - ~300 discrete ordinates or 1M-1B MC particles
  - ~200 frequency groups
  - 100s of timesteps
- Equals lots of unknowns, lots of operations

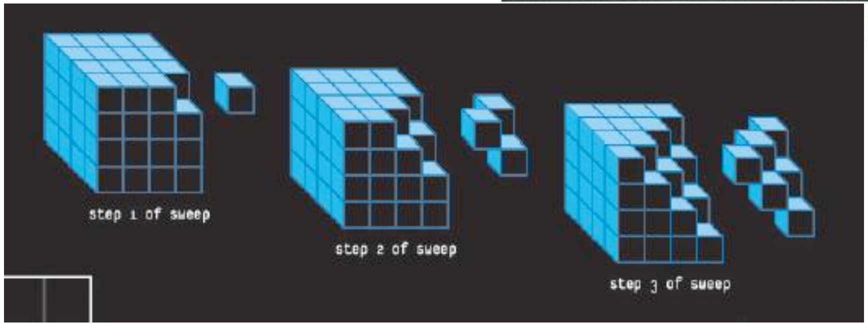
CCS-4 Software Products

- Linear transport of neutrons and gammas
  - **PARTISN**: deterministic S_N on Block AMR meshes
- Nonlinear transport of thermal x-rays
  - **Milagro**: Implicit Monte Carlo (IMC) on AMR (Jayenne Project)
  - **Serrano**: S_N for XY, RZ, R, and slab geometries on unstructured meshes (Capsaicin Project)
  - **Zathras**: diffusion and P1 on multi-geometry, multi-dimensional AMR meshes

PARTISN (PARallel TIme-dependent SN): neutron and gamma ray transport

- Available through RSICC (Radiation Safety Information Computational Center)
- S_N (discrete ordinates)
- Multi-dimensional
- Multi-geometry
- Block Adaptive Mesh Refinement (AMR) Meshes
- Parallel





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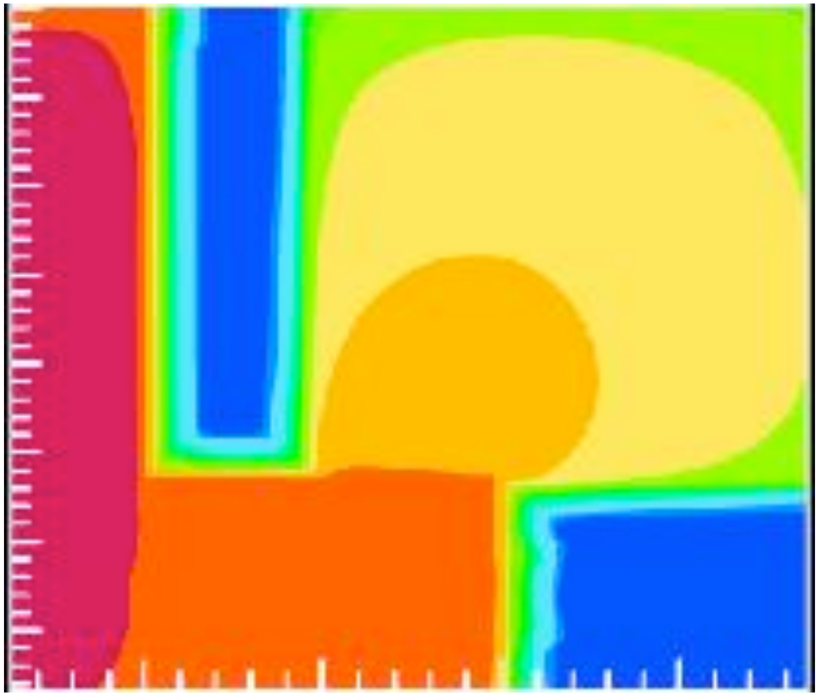
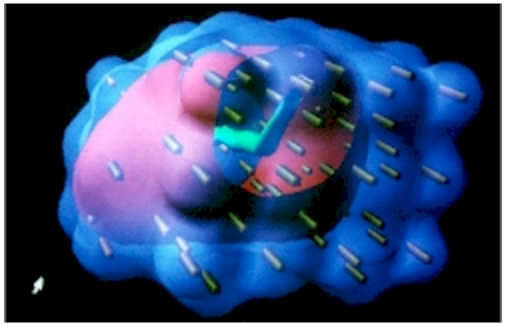
Jon Dahl

Radiation Transport Applications: Shielding simulations by PARTISN

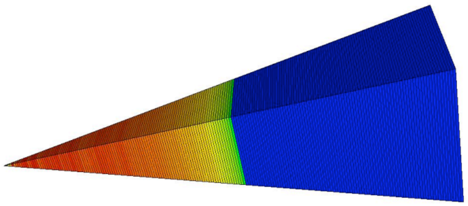


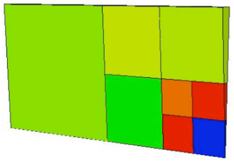
Radiation Transport Applications: Brachytherapy Cancer Treatment

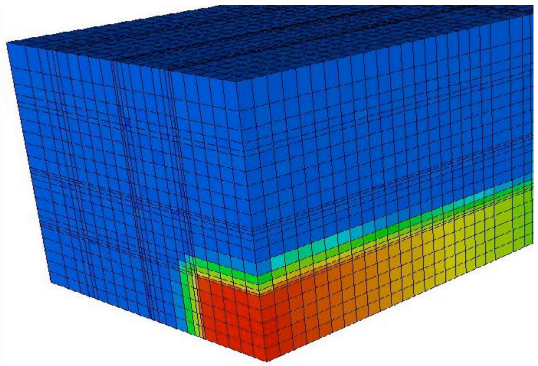


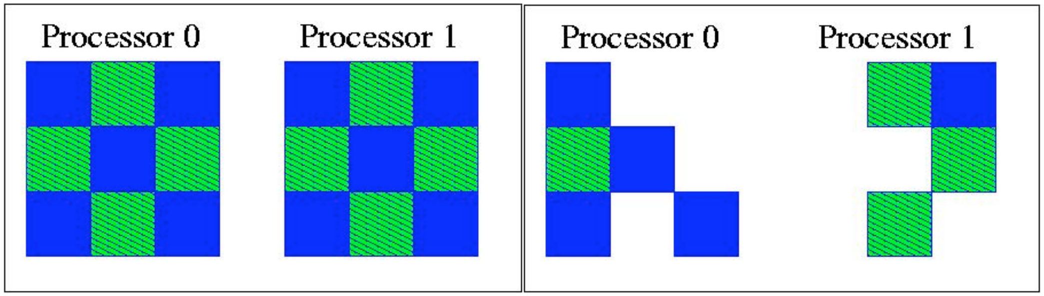
Milagro IMC for thermal x-ray transport

- Multi-dimension, AMR meshes
- Fleck & Cummings time-implicitness
- Object-oriented C++ with template parameterization of independent variables (e.g., mesh types)
- Parallel: mesh replication or mesh decomposition









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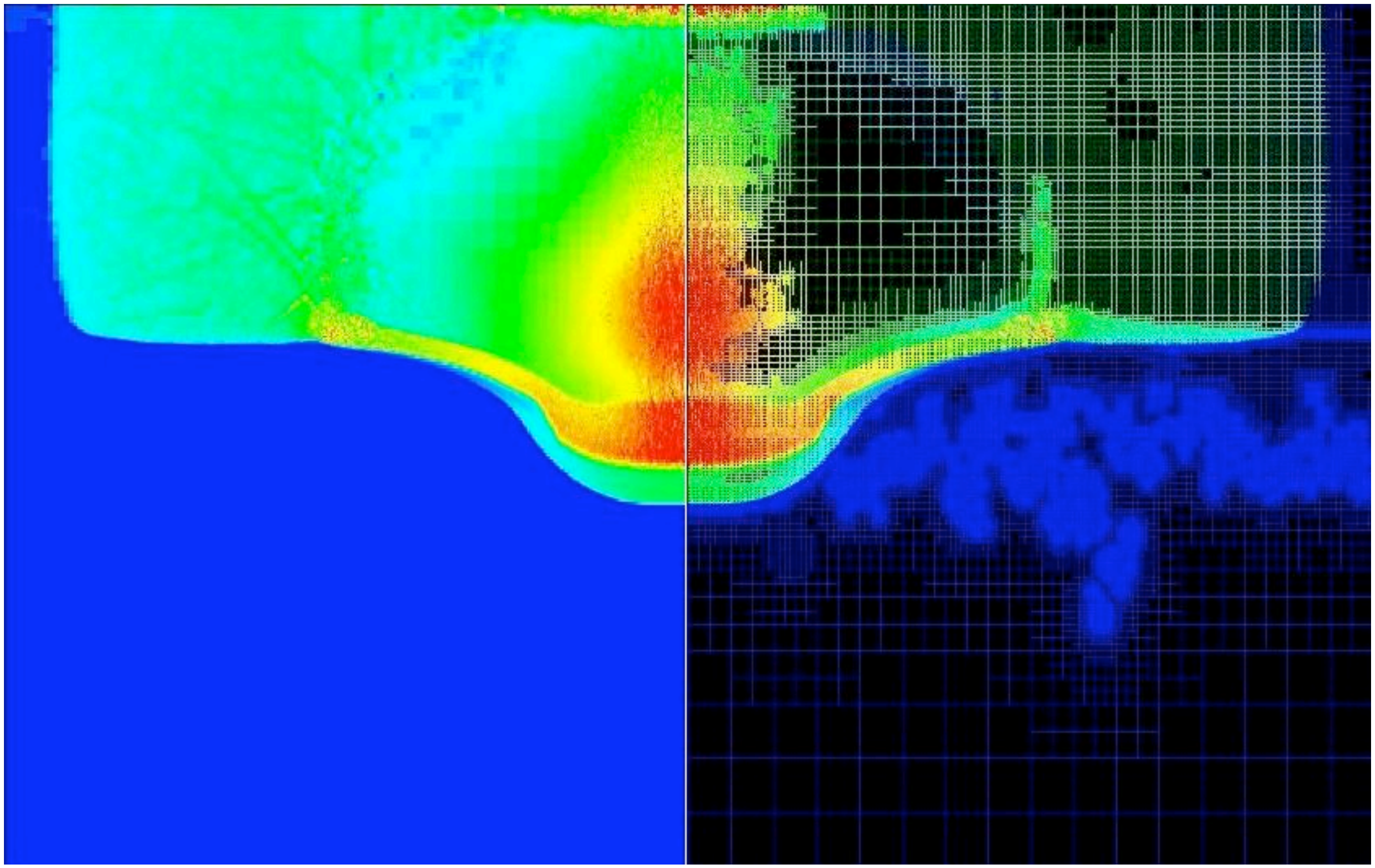
Radiation Transport Applications: Hot comet impacting a granite planet



Radiation temperature

IMC Simulation

Density

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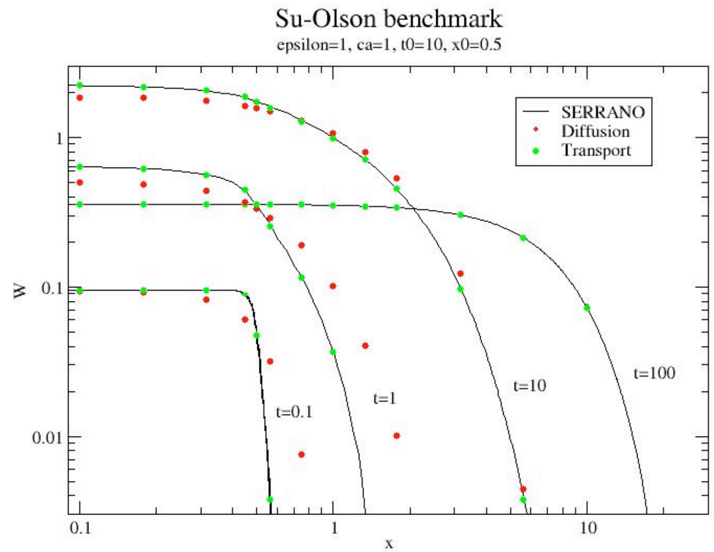
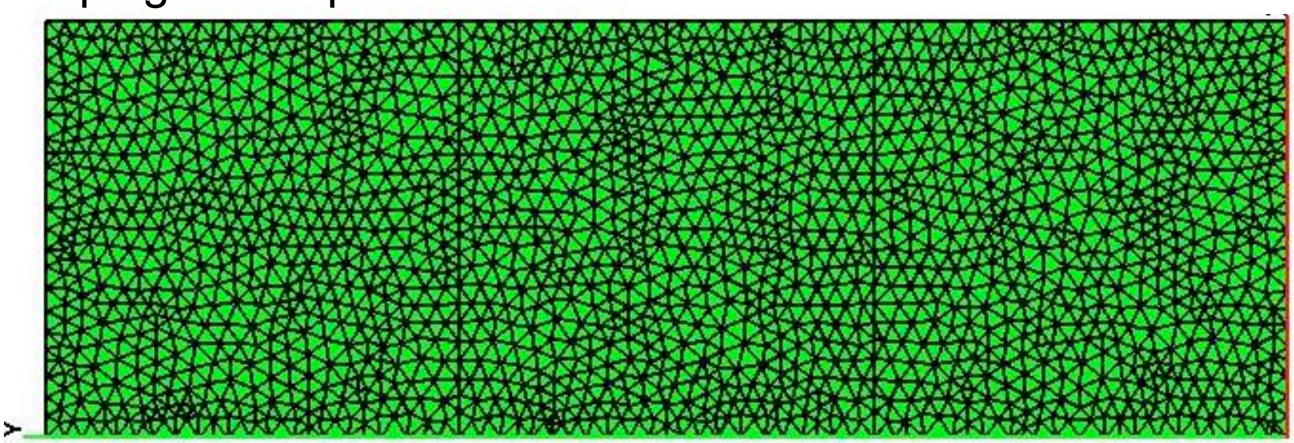
Serrano
for thermal x-ray transport

Kelly Thompson, Jae Chang,
Jim Warsa, Kent Budge

- XY, RZ, slab and spherical geometries
- Unstructured meshes
- Parallel
  - domain decomposition
  - Full sweeps or inexact block Jacobi
- Discontinuous Finite Element
- Synthetic Acceleration (TSA, DSA)
- Advanced lumping techniques

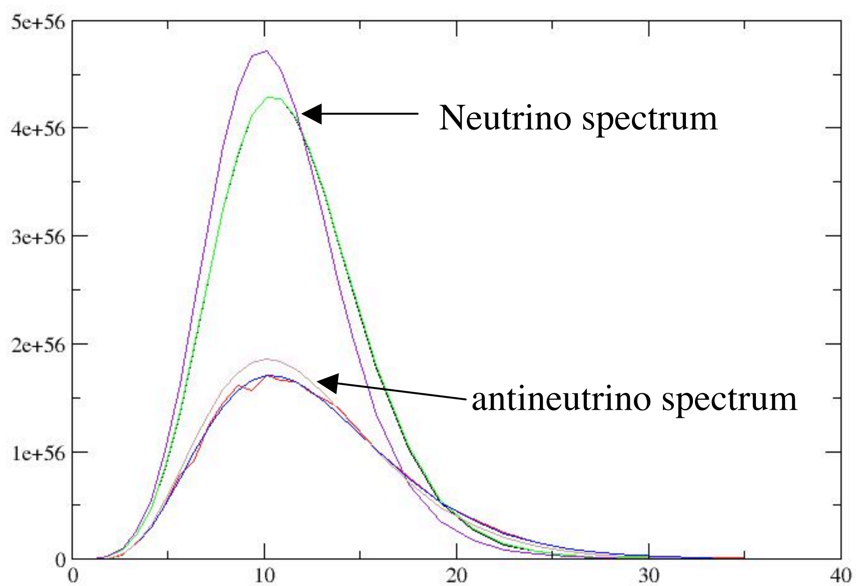




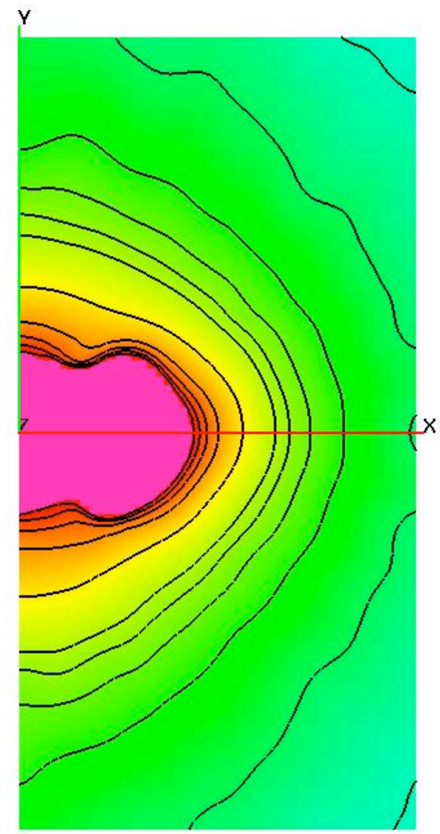
Kent Budge

Serrano software is being used to simulate neutrino transport in supernova

- Shown is the emergent spectrum of neutrinos and antineutrinos from a collapsing supernova.
- S_N and Monte Carlo results agree.
- Flux-limited diffusion results are higher and shifted to lower energy.



Neutrino energy density



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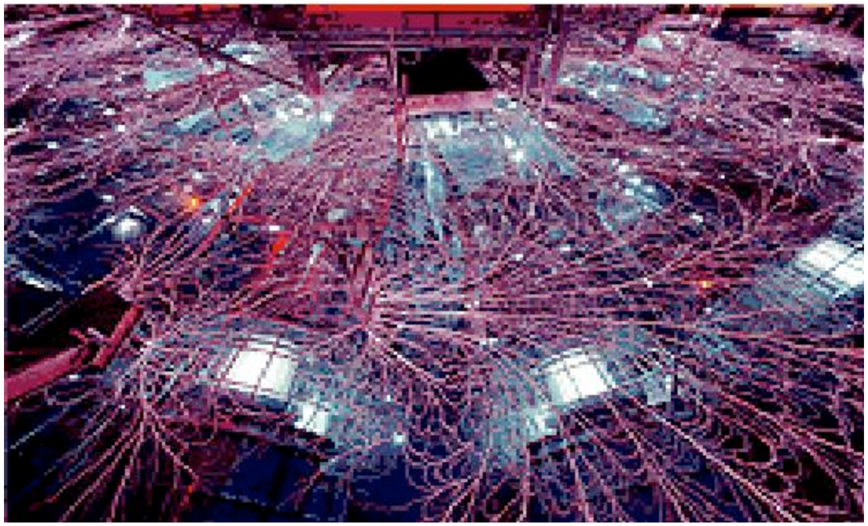
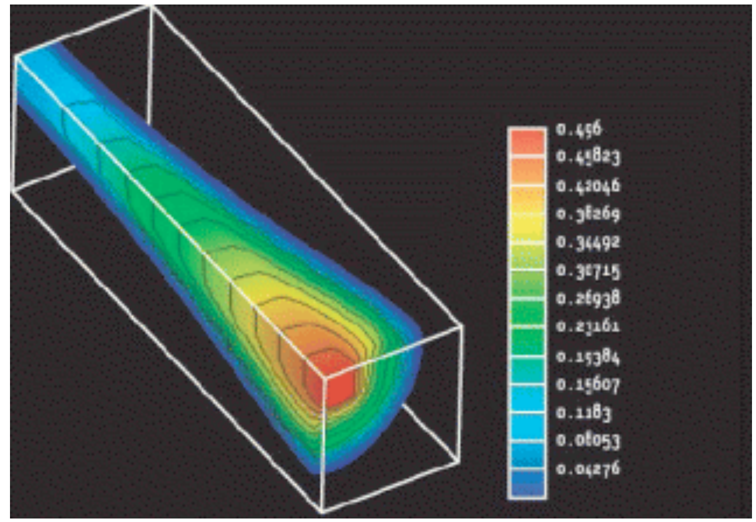
Radiation Transport Applications: Z-Pinch Machine at Sandia National Lab

Scott Turner
Mike Hall, CCS-2
Mark Gray



Zathras diffusion simulation

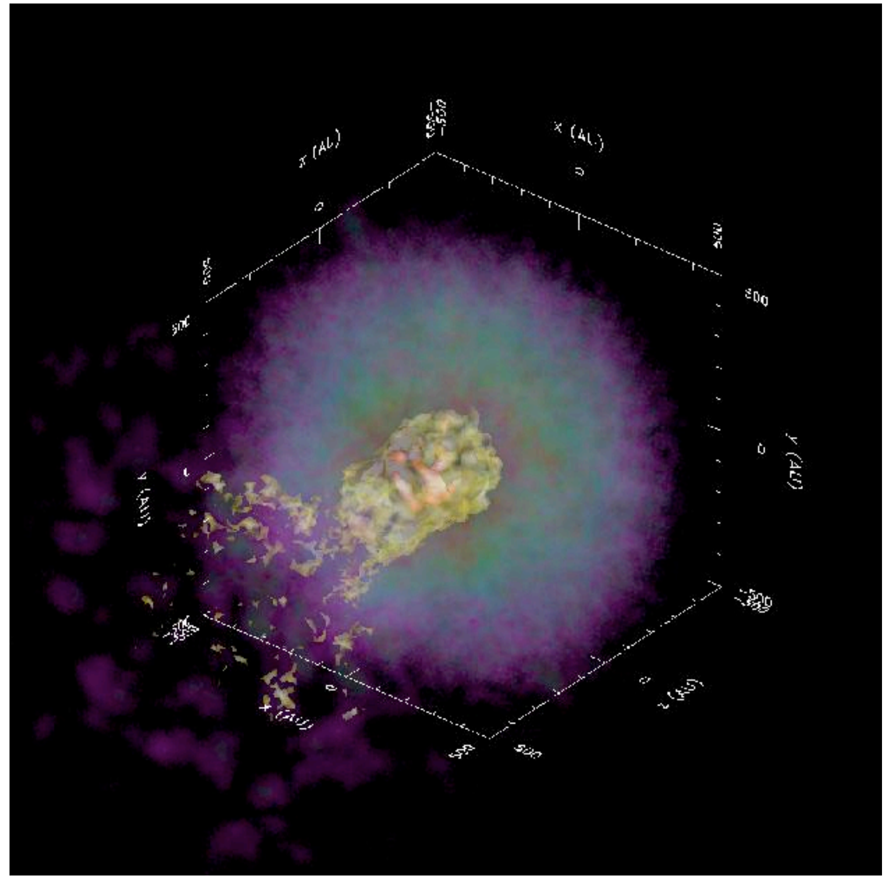


Electrical discharges illuminate the surface of the Z machine, the world's most powerful X-ray source, during a recent accelerator shot. By early 1998, the Sandia National Laboratories accelerator had achieved temperatures of 1.8 million degrees, close to the 2 to 3 million degrees required for nuclear fusion. Breakthroughs have enabled the machine to increase its power output roughly seven times. (Photo by Randy Montoya)

Aimee Hungerford

Radiation Transport Applications: Astrophysics

- Asymmetric supernova explosion
- Produces brighter radioactive decay lines than symmetric
- Linear post-process Monte Carlo transport
- Nonlinear, fully coupled transport in the future



Radiation Transport Issues

- Discretization for 2D/3D polygonal/polyhedral cells
- Stability, lack of stability, and stability analysis
- Too much memory usage
- Too slow
- Accuracy not always guaranteed
- Slow convergence
- You want issues, we’ve got even more issues….

Activities in Support of Methods and Algorithms R&D

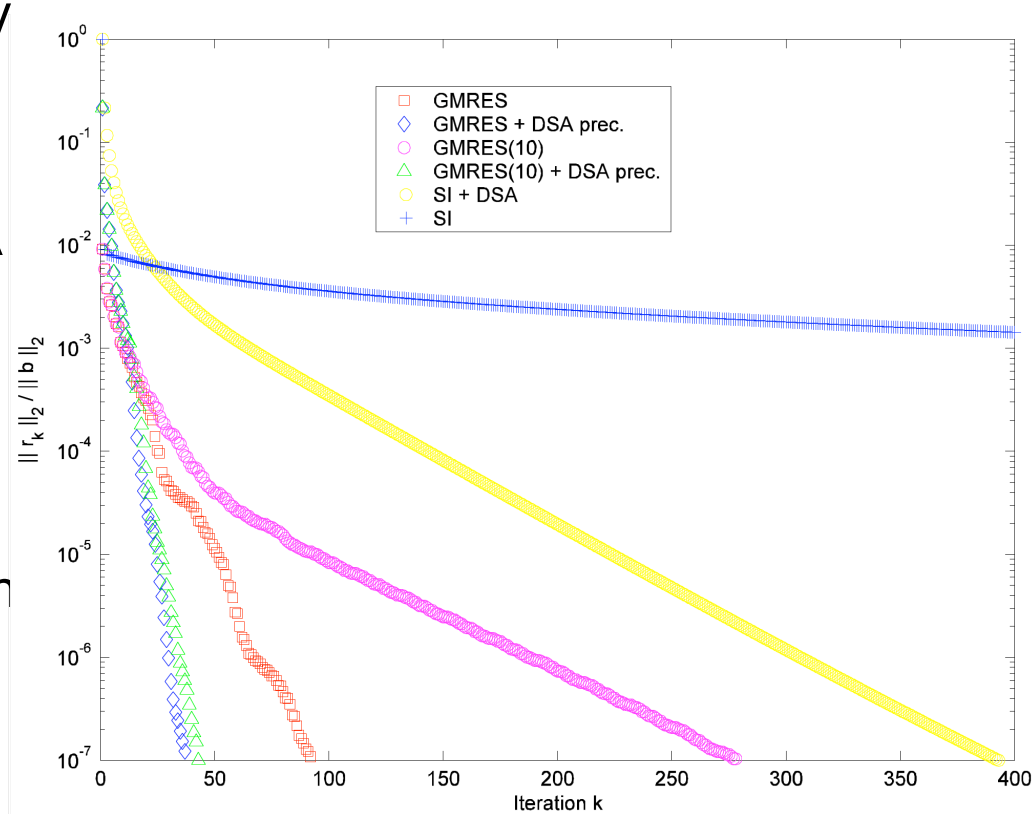
- Research by TSMs: Programmatic, WSR, LDRD
- Summer students
- Journal Club
- University contracts
  - University of Michigan
  - University of New Mexico
  - Pennsylvania State University
  - Oregon State University
- Publishing, Conferences, Workshops
  - American Nuclear Society, SIAM, APS, NEDCD, …
- Collaborations
  - E.g., May 22-24, 2006: Technical exchange with visiting delegation from the Russian VNIIEF laboratory. Topics: transport, hydro, computer architectures, parallel computing.

Radiation Transport Research

- Deterministic Transport
  - Discretizations of transport/acceleration on unstructured meshes
  - Lumping
  - Diffusion/Transport Synthetic Acceleration (DSA and TSA)
  - Krylov subspace methods with DSA as a preconditioner
  - Parallel implementations
  - Moving material methods
- Stochastic Transport
  - Hybrid methods
  - Residual Monte Carlo methods
  - General data decomposition parallel schemes

Krylov Iterative Methods

- Huge advance in deterministic transport (early 1990s-now).
- Obviates the need for consistency when TSA/DSA is used a preconditioner.
- Even without TSA/DSA, Krylov methods improve convergence rates over Source Iteration (Richardson Iteration)



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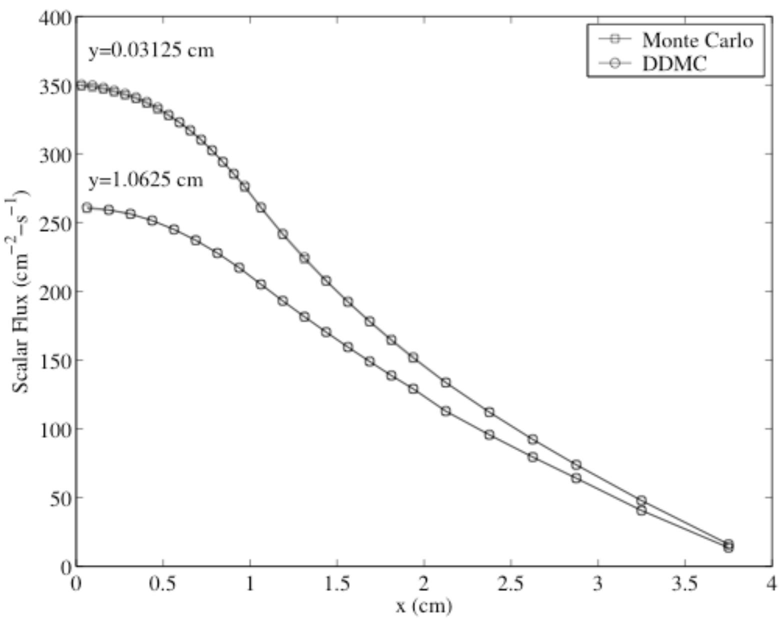
Hybrid Monte Carlo: Discrete Diffusion Monte Carlo (DDMC)

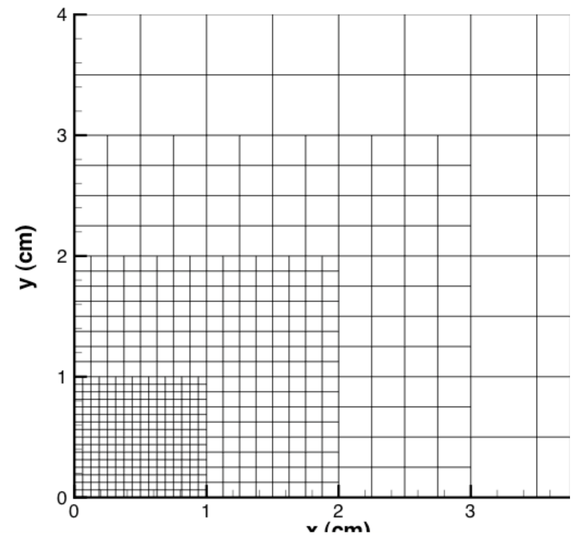
- Particle-based method recently extended to thermal x-ray transport
- Spatial cells are kernels of various flavors
  - Spatially continuous Monte Carlo transport
  - Cell-centered diffusion
  - Deterministic, lumped linear discontinuous
- Use diffusion in phase-space regions where you can; transport where you must
- Speedups of up to 1000s
- Fully time-consistent
- Latest research
  - Correct asymptotic behavior at transport-diffusion interfaces
    - Densmore, Jeffery D., Interface methods for hybrid Monte Carlo-diffusion radiation-transport simulations, Annals of Nuclear Energy, Volume: 33, Issue: 4, March, 2006, pp. 343-353
  - AMR meshes in 2-D XY
- Future research
  - Capturing transient regimes in time at transport-diffusion interfaces
  - Incorporating frequency into the phase-space decomposition

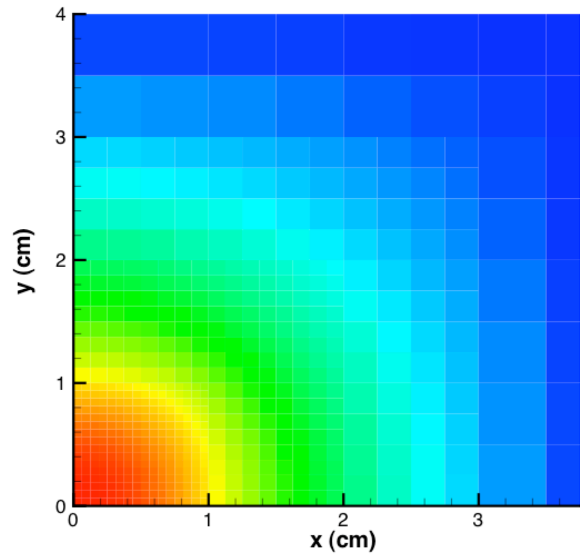
Jeff Densmore

Discrete Diffusion Monte Carlo (DDMC): linear transport on 2-D AMR Meshes

- Speedup of 180 over stock Monte Carlo



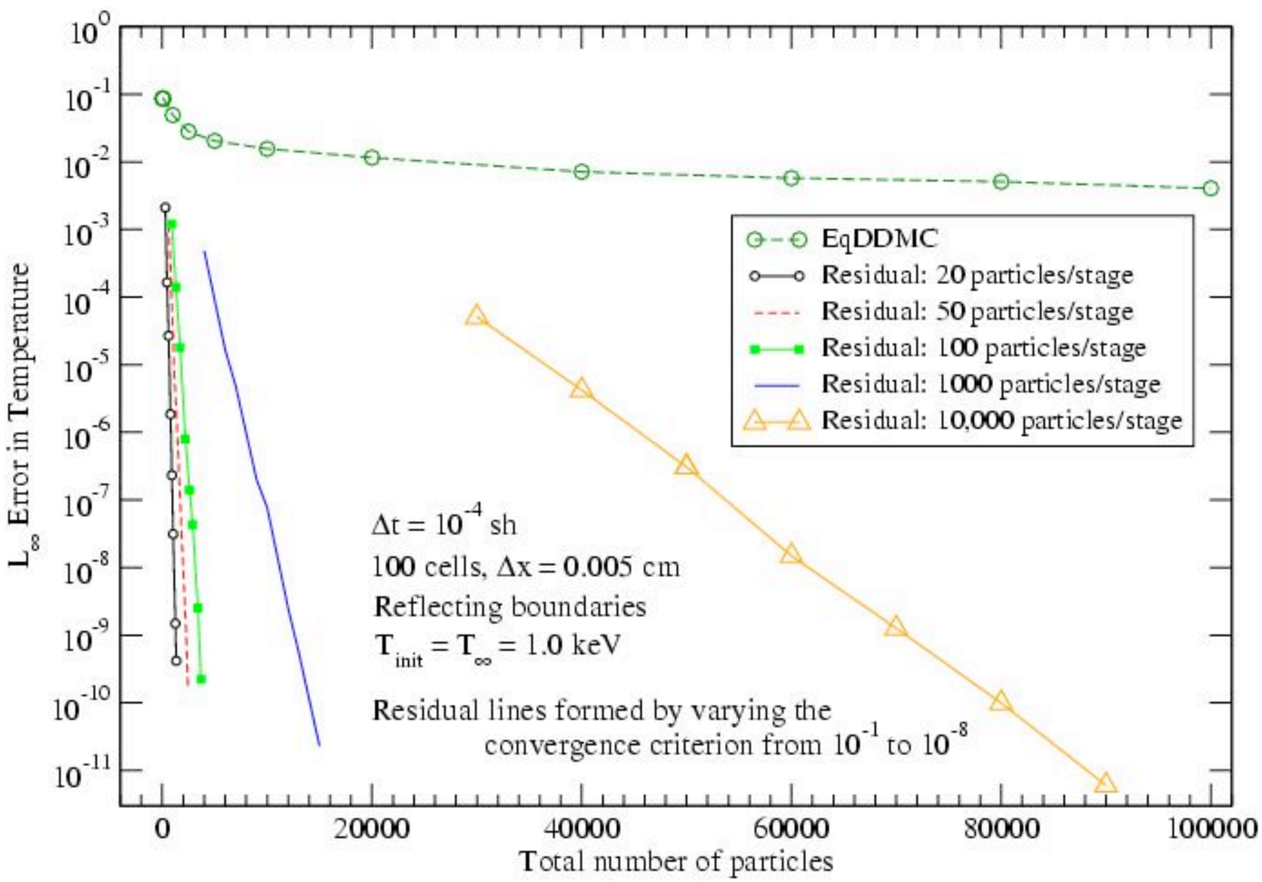




Residual Monte Carlo (ala Halton)

- The method for solving Ax=b is the same as for solving $A\delta x=r$, where $\delta x=x-x'$, x' is an approximation to x, and the residual $r=b-Ax'$.
- We apply it to one of our hybrid methods, the Discrete Diffusion Monte Carlo method:
  - Start with solution estimate, x'
  - Perform stages until convergence
    - Use conventional MC to solve residual eq.
    - Update: $x' \leftarrow x' + \delta x$
  - Iterate nonlinearities if desired
- Evans, T.M. ; Urbatsch, T.J. ; Lichtenstein, H. ; Morel, J.E., "A residual Monte Carlo method for discrete thermal radiative diffusion," Journal of Computational Physics, Volume: 189, Issue: 2, August 10, 2003, pp. 539-556.

Residual Monte Carlo: Exponential Convergence



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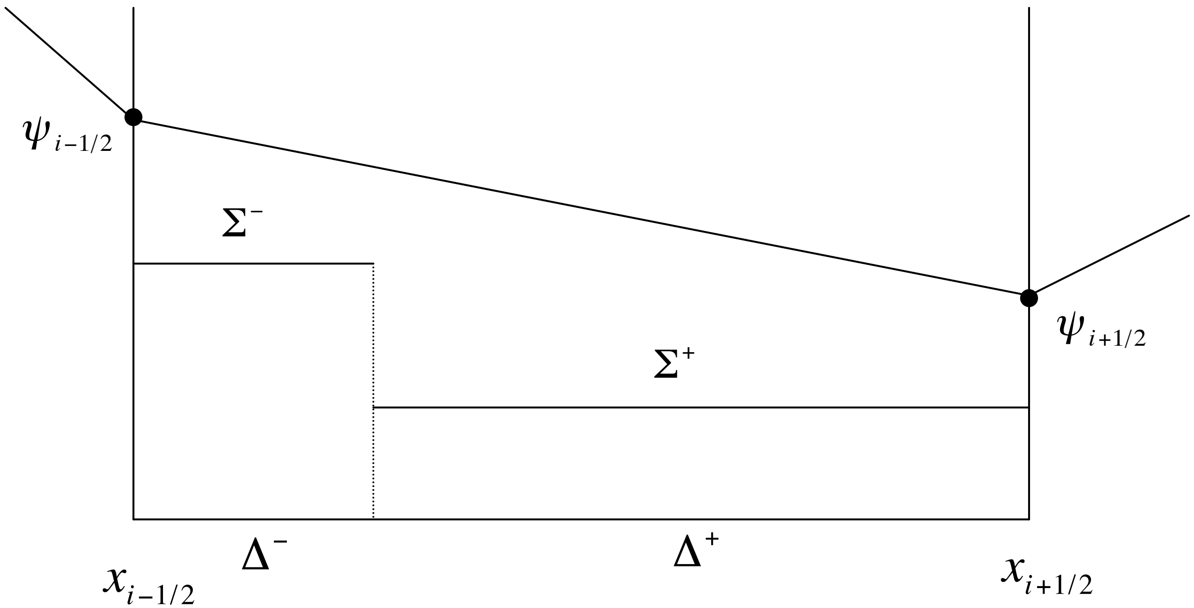
Ed Larsen, U Mich
Randy Baker, CCS-4

Research in Progress: Sub-cell treatments in PARTISN

- Consider a material interface within a cell in 1D planar geometry



$$\Delta = \Delta^- + \Delta^+$$

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Ed Larsen, U Mich
Randy Baker, CCS-4

Research in Progress: Sub-cell treatments in PARTISN

- The Diamond Difference method has the following closure,

$$\psi_i = \frac{\psi_{i-1/2} + \psi_{i+1/2}}{2}$$

- Then, traditionally, in heterogeneous cells, cross sections are **volume-weighted**,

$$\frac{1}{\Delta}\int_{\Delta} \Sigma(x)\psi(x)dx = \psi_i \frac{1}{\Delta}\int_{\Delta} \Sigma(x)dx$$

$$= \frac{\Sigma^- \Delta^- + \Sigma^+ \Delta^+}{\Delta^- + \Delta^+}\psi_i$$

$$= \bar{\Sigma}\psi_i$$

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Ed Larsen, U Mich
Randy Baker, CCS-4

Research in Progress: Sub-cell treatments in PARTISN

- Ed Larsen, University of Michigan, derived a generalized Diamond Difference equation assuming a linear continuous representation of ψ.

$$\psi(x) = \psi_{i-1/2}\left(\frac{x_{i+1/2} - x}{\Delta}\right) + \psi_{i+1/2}\left(\frac{x - x_{i-1/2}}{\Delta}\right)$$

which results in a **flux-weighted average** of the cross sections

$$\frac{1}{\Delta}\int_{\Delta}\Sigma(x)\psi(x)dx = \frac{1}{2}\left(\psi_{i-1/2}\bar{\Sigma}^{-} + \psi_{i+1/2}\bar{\Sigma}^{+}\right)$$

$$= \frac{\Sigma^{-}\Delta^{-} + \Sigma^{+}\Delta^{+}}{\Delta}\psi_{i} + \frac{\left(\Sigma^{+} - \Sigma^{-}\right)\Delta^{-}\Delta^{+}}{\Delta^{2}}\frac{\left(\psi_{i+1/2} - \psi_{i-1/2}\right)}{2}$$

where

$$\bar{\Sigma}^{-} = \Sigma^{-}\left[1 - \left(\frac{\Delta^{+}}{\Delta}\right)^{2}\right] + \Sigma^{+}\left(\frac{\Delta^{+}}{\Delta}\right)^{2} \qquad \bar{\Sigma}^{+} = \Sigma^{-}\left(\frac{\Delta^{-}}{\Delta}\right)^{2} + \Sigma^{+}\left[1 - \left(\frac{\Delta^{-}}{\Delta}\right)^{2}\right]$$

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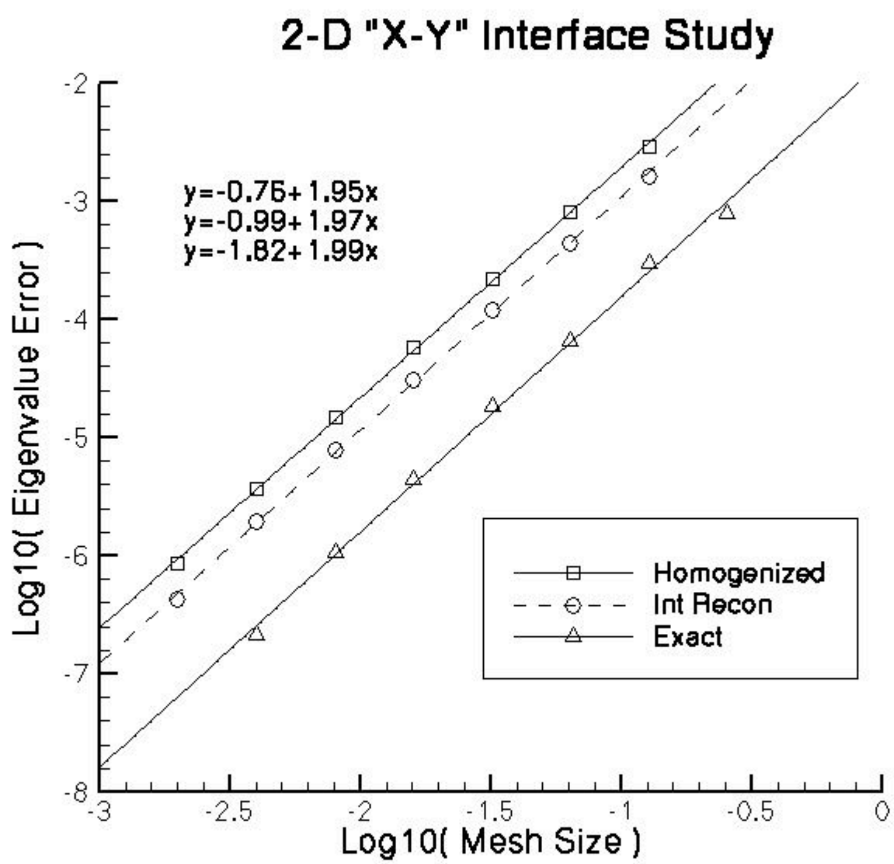
Randy Baker, CCS-4
Ed Larsen, Umich

Research in Progress: Sub-cell treatments in PARTISN

- Sub-grid representation is more accurate than traditional volume averaging
- Does not affect the order of spatial convergence



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Tim Kelley, CCS-4
Paul Henning, CCS-2
Ken Koch, CCS-DO

Advanced Architectures
Roadrunner

- We are porting our codes to new architectures with hierarchical memory models, such as IBM's Cell with SMPs and vector "accelerator" processors.
- First task is to hit hot spots. LANL's Roadrunner Project's Transport SWAT team has shown order-of-magnitude speedups in a part of Milagro IMC's source calculation.
- Next step will be to see if algorithm changes or entirely new algorithms will better utilize these new architectures.
- Instead of increasing the speed, we may wish to consider retaining current simulation speeds but using the vector processors to improve accuracy. A possibility may be to relegate sub-grid calculations to the vector processors. Improved nonlinearity treatment during an IMC time step could involve EOS table inversions, which the vector processors could handle.

Overview of Software Development Processes

In addition to configuration management, requirements management, integral testing and documentation, some other processes and practices:

- Design
  - component-based
  - levelized design
  - template concepts
  - reuse
- Documentation Templates
  - Vision and Scope
  - Bug Post-Mortems
- Testing
  - Repeatable (automatic and on-demand)
  - Unit
  - Integral
  - Shunt

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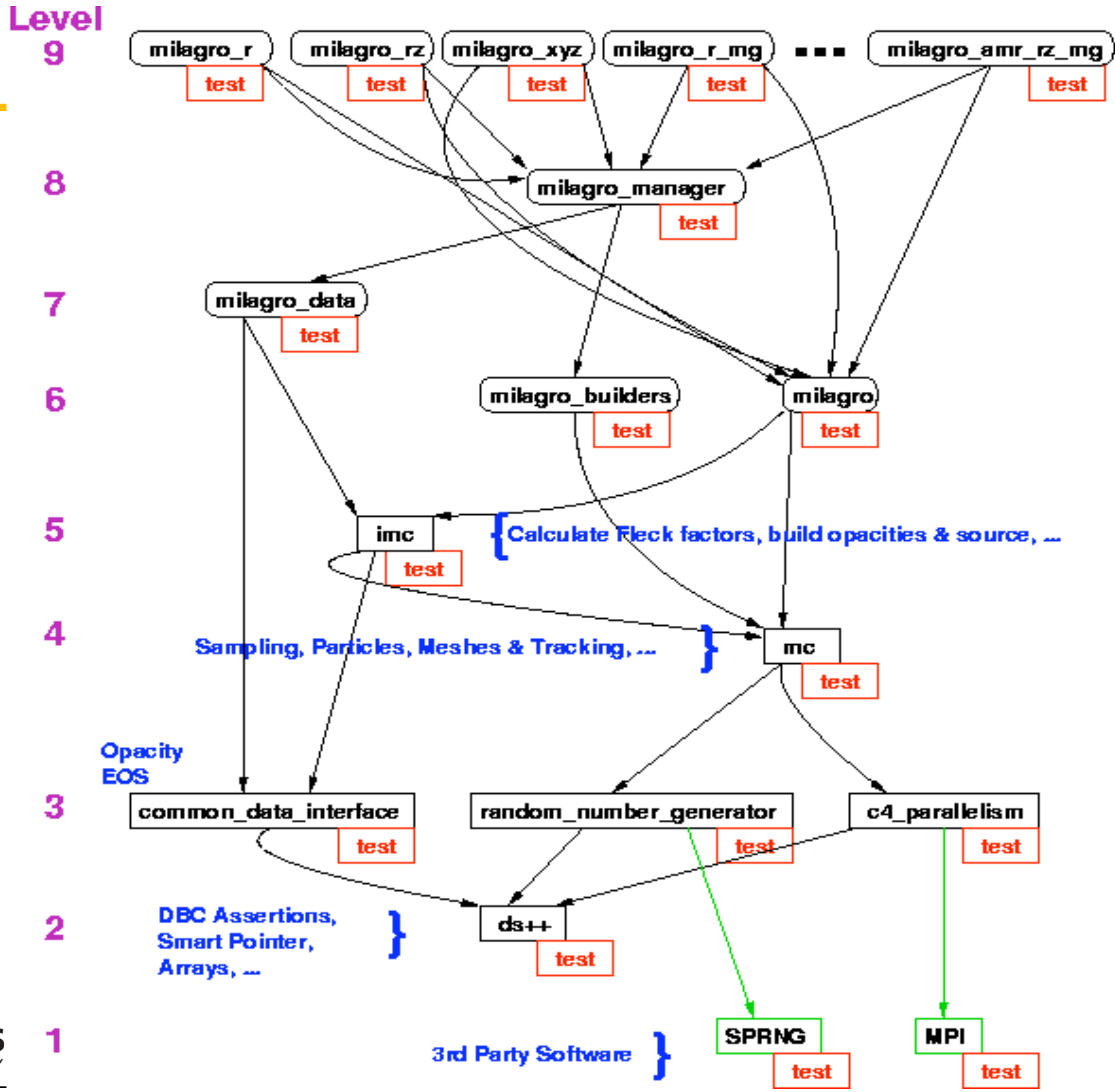
Milagro's Levelized Design



Example of Design-by-Contract (DBC)

DBC: Macros for selectively switching C++ assertions on and off

```
//! Find a frequency group, in [1,G], given a frequency [keV]
int find_group_given_a_freq(const double hnu) const
{
    // Require a valid frequency
    Require (hnu >= 0);

    // Make sure it's multigroup
    Check (group_boundaries.size() > 1);

    ……do binary search, with embedded Checks, to find group……

    // check that the group actually contains the frequency
    Ensure (hnu >= get_group_boundaries(group).first);
    Ensure (hnu <= get_group_boundaries(group).second);

    // return the group number in [1,G]
    return group;
}
```

Turn on during development, testing, and debugging

Turn off for production
--compile time switch
--no cpu time cost

"Buggy Pageant"
A Contest to Locate Code Defects

- This is a contest between two code teams to see how easily they can locate bugs in their codes.
  - Use compilers, linkers, DBC, tests, and, as a last resort, debuggers to find defects.
- The bugs are intended to represent defects inadvertently introduced by a developer on the team.
  - Cannot use "cvs" or "diff" or "ls -lart" to detect the defects introduced by the opposing team.
- Each team introduces defects in the *other* team's code.
- Contest is for each team to find the defects in their own code.
- Point system determines the winner.

A few of the bugs from previous "Buggy Pageant" demonstrations

- All random numbers were set to 1/2.
- Switched the value of the speed of light (c) and the radiation constant (a).
- Changed $\sin\theta$ to $\sin\phi$ in Ω_z when scattering from $\underline{\Omega}'$ to $\underline{\Omega}$ through (θ,ϕ).
- Switch scattering and absorption opacities
- Off-by-one (smaller) in broadcast of mesh
- Units error in the internal energy: g to kg in the heat capacity

In two different Buggy Pageant demonstrations, the average time for Tom Evans and a team of Tom Evans, Jeff Densmore, and Scott Mosher to find one of these bugs was 13.3 minutes!

CCS-4 will be well represented at the American Nuclear Society's Winter Meeting

- "Numerical Solution Algorithms for a P_{N-1}-Equivalent S_N Angular Discretization of the Transport Equation in One-Dimensional Spherical Geometry," James Warsa and Jim Morel (Texas A&M).
- "An Asymptotic-Preserving Lumped Bilinear-Discontinuous Spatial Finite Element Method for the Linearized Boltzmann Transport Equation," Jim Morel (Texas A&M) and James Warsa.
- "A Finite Element Transport Method for Spatial Cells with Material Interfaces," Randal S. Baker and Edward W. Larsen (University of Michigan).
- "Discrete Diffusion Monte Carlo for XY Adaptive Mesh Refinement-Style Meshes," Jeff Densmore, Tom Evans, and Mike Buksas.
- "Implicit Monte Carlo Methods for Three-Temperature Transport," Tom Evans and Jeff Densmore.
- "Time-Absorption Eigenvalue Searches Using Diffusion Synthetic Acceleration," Jon A. Dahl and Raymond E. Alcouffe.
- "Exact Solution of a Nonlinear, Time-Dependent, Infinite-Medium, Grey Radiative Transfer Problem," Scott W. Mosher.

2006 Students

- **Massimiliano Rosa**, The Pennsylvania State University, “Fourier analysis of parallel, inexact block-jacobi solution technique to solve the transport equation with transport synthetic acceleration (TSA) diffusion synthetic acceleration (DSA) in 2D geometry,” mentor Jae Chang.
- **Alexander Maslowski**, Texas A&M, DOE Nuclear Engineering Health Physics Fellowship, ”Practical approximations to general relativistic effects in neutrino transport,” mentor Kent Budge.
- **Teresa Bailey**, Texas A&M, DOE Computational Science Fellow, “Analysis of Piecewise Linear Discontinuous and Upwind Corner Balance spatial discretization schemes for 2D transport,” mentor Kelly Thompson.
- **Michael Reed**, Texas A&M, "Finite Element Transport Discretization Schemes That Include Material Interfaces Within Spatial Cells,” mentor Randy Baker.
- **Erin Fichtl**, UNM, "Iterative methods for radiation transport in binary stochastic media," mentor Jim Warsa.
- **Rick Gleicher**, UNM, "Cell-Local Global Discontinuous Finite Element Spatial Discretizations on Polygons for the Two-Dimensional SN Transport Equation," mentor Jim Warsa.
- **Eric Baker**, Oregon State University, "Software Development for the generation of Quadruple Range Multi-dimensional Quadrature Sets," mentor Jon Dahl.

CCS-4's current and potential interactions with other groups in CCS

- CCS-1
  - kind of non-existent now, except indirectly through
    - the systems and products CCS-1 researches, develops, and deploys
    - Roadrunner
  - Hope to strengthen the relationship by having the entertaining Ron Minnich talk to our group.
    - Tighten feedback loop between the two groups' products via shared unit tests and pre-release testing
    - Research on fault-tolerant algorithms
    - Research on algorithm-specific efficiency improvements

CCS-4's current and potential interactions with other groups in CCS

- CCS-2
  - Radiation-hydrodynamics methods, analysis, and applications
  - Algorithms for advanced architectures; Roadrunner
  - Bridging the gap between transport and the animation industry
  - Global Nuclear Energy Partnership
  - Programmatic efforts
- CCS-3
  - Performance modeling of CCS-4's algorithms
  - Potential to incorporate the detailed serial performance model of our IMC software into CCS-3's overall performance models
  - Monte Carlo methods research
  - Machine Learning

CCS-4's current and potential interactions with other groups in CCS

- CCS-5
  - Can we incorporate our neutron/gamma transport code, PARTISN, into TRANSIMS for homeland security---at least for benchmarking purposes?
- CCS-6
  - Past collaborations produced algorithms in MCNP that indicated the quality of sampling for criticality calculations. Can we extend this to our thermal X-ray transport software?
  - Application of Bayesian models to our algorithms?
    - Sensitivity of methods on physical data.
    - How deep can we embed Bayesian models into our transport methods?
      - Timestep control?
      - IMC in operator-split radiation-hydrodynamics?
      - Down to the detailed particle tracking in Monte Carlo?

Extra slides

Coupling multiple physics

- Loose coupling, such as post-process
  - Sufficient for loosely coupled physics
  - Do the next generation nuclear reactors qualify?
- Operator split for high energy density rad-hydro
  - Hydrodynamics, ICF material energy sources, thermal radiation
  - Time step control must be applied to each split
    - analogous to variance reduction in linear Monte Carlo transport, in that you can't recover from sufficiently large variance
  - Wrong order of operations can render time-implicitness useless
  - Correct order of operations can serve to better couple the splits
    - Closer to unsplit accuracy without the unsplit cost
- Unsplit
  - Newton-Krylov possible for diffusion and hydrodynamics/thermal hydraulics
  - Transport is still too memory- and cpu-cost prohibitive

Coupling multiple physics

Tom Evans

- Split material energy update

$$c_v \frac{T' - T^n}{\Delta t} = Q$$

$$\frac{E^{n+1} - E^n}{\Delta t} + f\sigma c E^{n+1} = f\sigma c a T'^4$$

$$c_v \frac{T^{n+1} - T'}{\Delta t} = f\sigma c\left(E - aT'^4\right)$$

- Unsplit material energy update couples in with the Fleck and Cummings IMC implicitness and allows for timesteps up to 10-100x bigger.

$$\frac{E^{n+1} - E^n}{\Delta t} + f\sigma c E^{n+1} = f\sigma c a T^{n4} + (1 - f)Q$$

$$c_v \frac{T^{n+1} - T'}{\Delta t} = f\sigma c\left(E - aT'^4\right) + fQ$$